# p-Hydroxymandelic acid, propionyl, DTFMBz

**Inchi:** InChI=1S/C23H20F6O6/c1-3-18(30)34-17-7-5-14(6-8-17)20(35-19(31)4-2)21(32)33-12-1
**InchiKey:** NLHBPFNXDVJVDB-UHFFFAOYSA-N
**Formula:** C23H20F6O6
**SMILES:** CCC(=O)Oc1ccc(C(OC(=O)CC)C(=O)OCc2cc(C(F)(F)F)cc(C(F)(F)F)c2)cc1
**Mol. weight [g/mol]:** 506.39

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1528.67 | kJ/mol | Joback Method |
| hf | -2013.24 | kJ/mol | Joback Method |
| hfus | 50.73 | kJ/mol | Joback Method |
| hvap | 92.92 | kJ/mol | Joback Method |
| log10ws | -7.18 | | Crippen Method |
| logp | 5.777 | | Crippen Method |
| mcvol | 320.350 | ml/mol | McGowan Method |
| pc | 1193.17 | kPa | Joback Method |
| rinpol | 2256.00 | | NIST Webbook |
| rinpol | 2256.00 | | NIST Webbook |
| tb | 1011.53 | K | Joback Method |
| tc | 1238.49 | K | Joback Method |
| tf | 649.23 | K | Joback Method |
| vc | 1.260 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1031.49 | J/mol×K | 1011.53 | Joback Method |
| cpg | 1041.40 | J/mol×K | 1049.36 | Joback Method |
| cpg | 1050.06 | J/mol×K | 1087.18 | Joback Method |
| cpg | 1057.54 | J/mol×K | 1125.01 | Joback Method |
| cpg | 1063.91 | J/mol×K | 1162.84 | Joback Method |
| cpg | 1069.24 | J/mol×K | 1200.66 | Joback Method |
| cpg | 1073.60 | J/mol×K | 1238.49 | Joback Method |

# Sources

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|---|---|
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R539009&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# Legend

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |